

# ***Demo: Creating the Calibration Curve and Processing Method 8261 Data (PC version)***

Michael H. Hiatt  
*U.S. Environmental Protection Agency  
National Exposure Research Laboratory  
Environmental Sciences Division  
P.O. Box 93478, Las Vegas, Nevada 89193-3478*

# ***Demonstration. Install SMCREPORTER***

- This slide show is in addition to documentation provided with method 8261 software.
- The software is available on this website  
<http://www.epa.gov/nerlesd1/chemistry/vacuum/methods/software-pc.htm>
- Download the zip file as per Installation Guide at the site (It is recommended to also download the Getting Started and User's Guide but not necessary for this exercise).
- You will have created a folder "SMCREPORTER" on the C drive as the default.



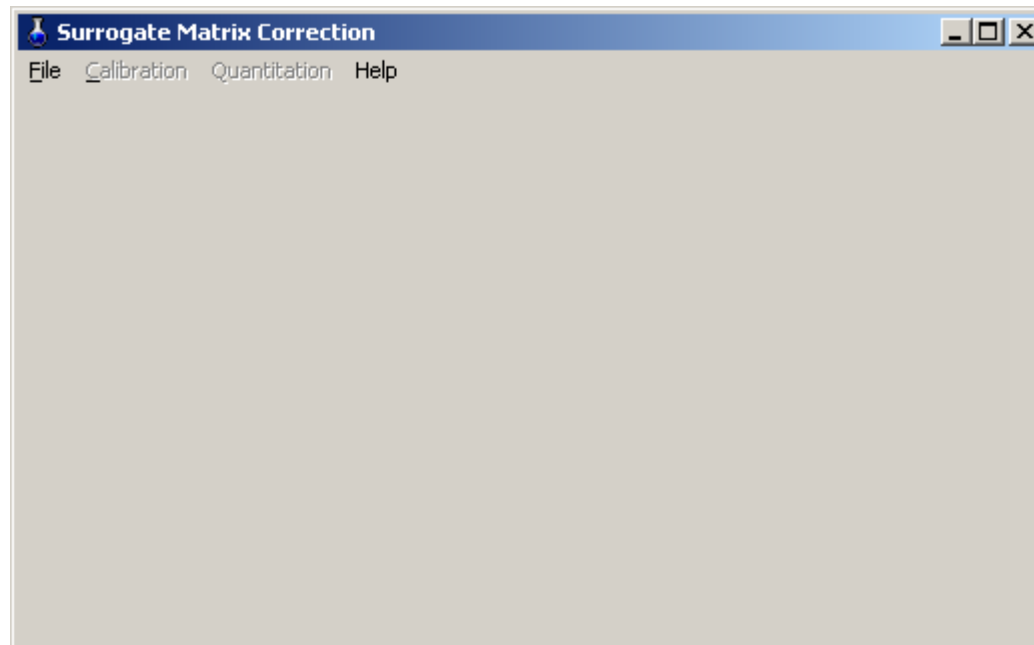
# *Load Demonstration Files for this Exercise*

- The reader can reproduce the processing to be presented by installing Smcreporter-Standalone and installing the data files used. Both can be installed from <http://www.epa.gov/nerlesd1/chemistry/vacuum/methods/default.htm>.
- If the software and data files are installed a new folder, SMCREPORTER, is created. Under the new folder a sub-folder Cal\_example contains the example data files including the method 8261 library (All.txt), surrogate file (surrogate.ini), blank (blank.txt), and five standards (StandardA through StandardE).
- **This presentation assumes an understanding of the method 8261 calculations using surrogates.** See <http://www.epa.gov/nerlesd1/chemistry/vacuum/reference/analysis/anal.htm>.



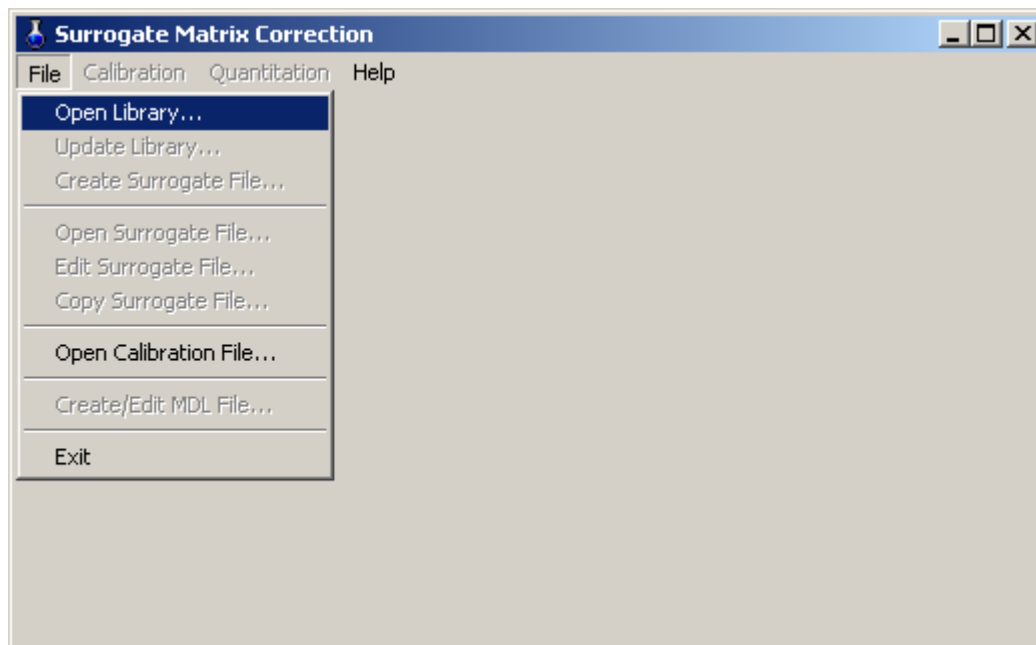
# *Run SmcReporter*

- Go to Windows->Programs->and click on SmcReporter. The following is displayed



# *Load Library “ALL.txt”*

- Go to File then “Open Library”

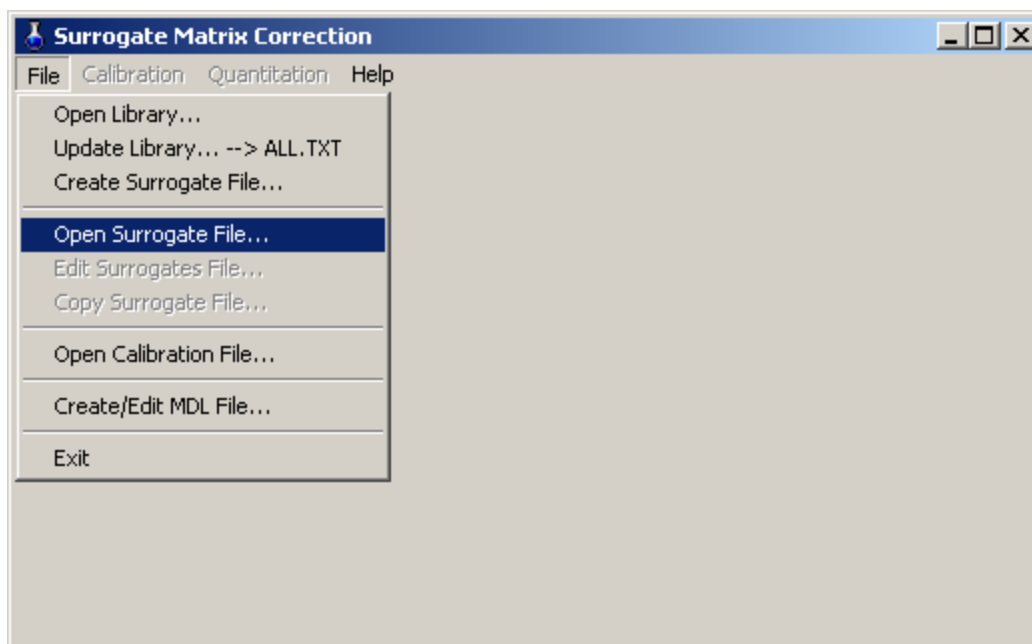


- Open File window is displayed. Navigate to the Cal\_example folder and highlight All.txt and Open. The “All” library is now activated.



# Load Surrogate File “surrogate.ini”

- Go to File then “Open Surrogate File”



- Open File window is displayed. Navigate to the Cal\_example folder and highlight surrogate.ini and Open. The surrogate file is activated.



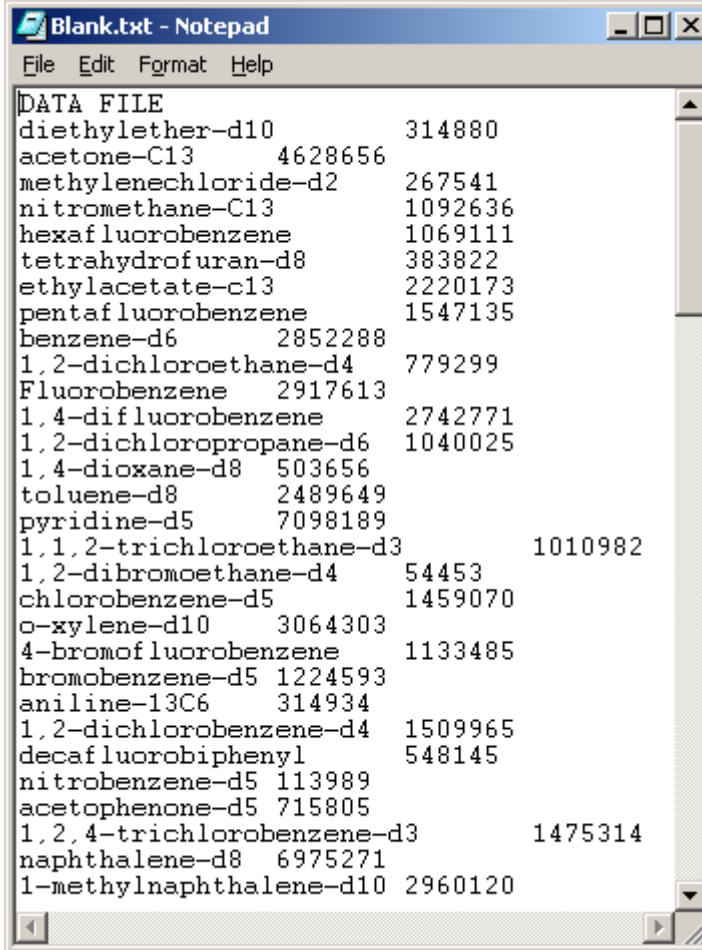
## *GC/MS data set*

- The PC version data must be in ASCII format and readable in Notepad (e.g. StandardA.txt)
- These data files contain the GC/MS response (area) for each compound.
- Each compound in the “All.txt” library must be present in the data file.
- The first line of the data file contains the label “DATA FILE”



# Data File Example

- Open the blank.txt data file in notepad
- Note each compound is identified with a GC/MS response tab delimited



```
Blank.txt - Notepad
File Edit Format Help
DATA FILE
diethylether-d10      314880
acetone-C13          4628656
methylenechloride-d2  267541
nitromethane-C13     1092636
hexafluorobenzene    1069111
tetrahydrofuran-d8  383822
ethylacetate-c13     2220173
pentafluorobenzene   1547135
benzene-d6           2852288
1,2-dichloroethane-d4 779299
Fluorobenzene        2917613
1,4-difluorobenzene  2742771
1,2-dichloropropane-d6 1040025
1,4-dioxane-d8       503656
toluene-d8           2489649
pyridine-d5          7098189
1,1,2-trichloroethane-d3 1010982
1,2-dibromoethane-d4  54453
chlorobenzene-d5      1459070
o-xylene-d10         3064303
4-bromofluorobenzene 1133485
bromobenzene-d5      1224593
aniline-13C6         314934
1,2-dichlorobenzene-d4 1509965
decafluorobiphenyl   548145
nitrobenzene-d5      113989
acetophenone-d5      715805
1,2,4-trichlorobenzene-d3 1475314
naphthalene-d8       6975271
1-methylnaphthalene-d10 2960120
```





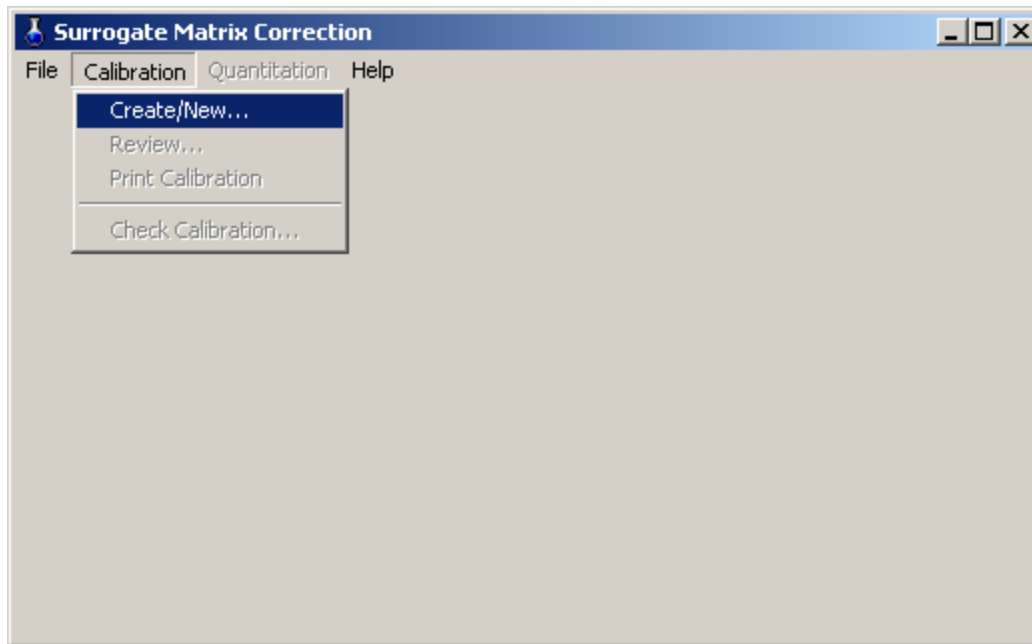
# Calibration

- The library and surrogate files represent the compounds in the surrogates and standards (see slide presentation “Running Samples”)
- Standards are prepared as in “Running Samples” slide presentation ([http://www.epa.gov/nerlesd1/chemistry/vacuum/training/pdf/run\\_samples.pdf](http://www.epa.gov/nerlesd1/chemistry/vacuum/training/pdf/run_samples.pdf)) with the exception the nitrogen containing compounds are 3X the amounts used in “Running Samples”.
- The standard amounts for Standards A through E are expressed as dilutions of conc1 in the All.txt library (the mass is by compound and not global)
- All runs contain 5 uL of the working surrogate solution and standards are as follows:
  - A. 5uL 1:1 working standard, Conc1 or dilution 1
  - B. 1uL 1:1 working standard, dilution 0.2
  - C. 5uL 1:10 working standard, dilution 0.1
  - D. 3uL 1:10 working standard, dilution 0.06
  - E. 1uL 1:10 working standard, dilution 0.02



# Creating the Calibration Curve for Data Processing

- Go to Calibration and select “Create/New”

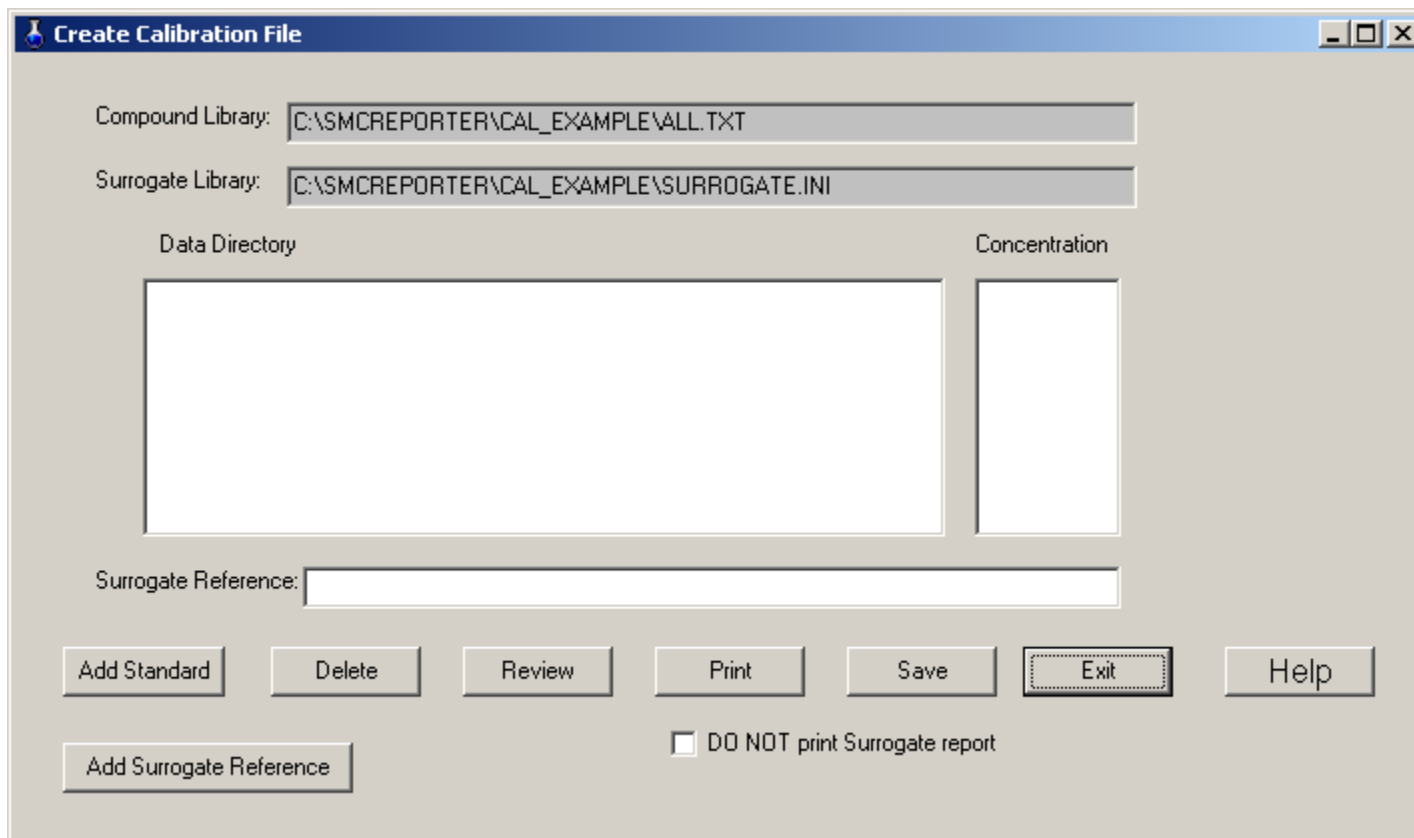


- A display indicates library and surrogate files that are going to be used for calibration. Verify “surrogate.ini” and select “OK”



# Create Calibration File

- The next window, “Create Calibration File” is then displayed.



The screenshot shows a Windows-style dialog box titled "Create Calibration File". It contains the following elements:

- Compound Library:** A text box containing the path "C:\SMCREPORTER\CAL\_EXAMPLE\ALL.TXT".
- Surrogate Library:** A text box containing the path "C:\SMCREPORTER\CAL\_EXAMPLE\SURROGATE.INI".
- Data Directory:** A large empty rectangular box.
- Concentration:** A smaller empty rectangular box.
- Surrogate Reference:** A text box.
- Buttons:** A row of buttons including "Add Standard", "Delete", "Review", "Print", "Save", "Exit" (highlighted with a dashed border), and "Help".
- Checkboxes:** A checkbox labeled "DO NOT print Surrogate report" which is currently unchecked.
- Additional Button:** An "Add Surrogate Reference" button located below the "Surrogate Reference" text box.



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# Surrogate Reference

- The surrogate reference used in calibration is a list of surrogates with their boiling points (BP's) and relative volatilities ( $\alpha$ ) and how these surrogates are to be used.
- Surrogates monitor variations and their responses are used to normalize standard's response factors.
- A surrogate reference file can be any of the runs used to generate a calibration.
- Typically the blank run (blank.txt) run prior to the calibration standards is used.
- Select “Add Surrogate Reference” and using the “Open” window that is displayed navigate to the Cal\_example folder and select blank.txt file.



# Create Calibration File with Surrogate Reference Added

- Click on “Add Standard.”

The screenshot shows a Windows-style dialog box titled "Create Calibration File". It contains the following fields and controls:

- Compound Library:** A text box containing "C:\SMCREPORTER\CAL\_EXAMPLE\ALL.TXT".
- Surrogate Library:** A text box containing "C:\SMCREPORTER\CAL\_EXAMPLE\SURROGATE.INI".
- Data Directory:** A large empty text box.
- Concentration:** A smaller empty text box.
- Surrogate Reference:** A text box containing "C:\SMCREPORTER\Cal\_example\blank.txt".
- Buttons:** A row of buttons including "Add Standard", "Delete", "Review", "Print", "Save", "Exit", and "Help".
- Checkboxes:** A checkbox labeled "DO NOT print Surrogate report" which is currently unchecked.
- Additional Button:** A button labeled "Add Surrogate Reference" located below the main row of buttons.

A large green arrow points from the left side of the dialog box to the "Add Standard" button.

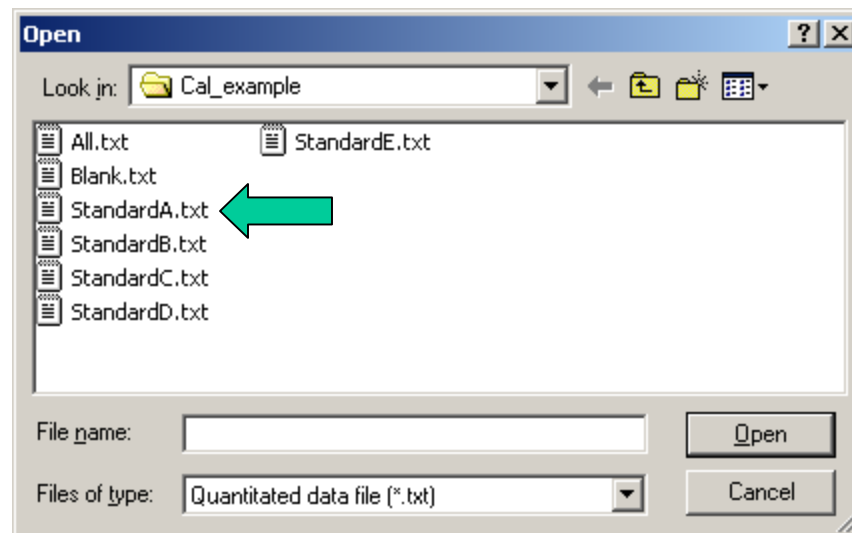


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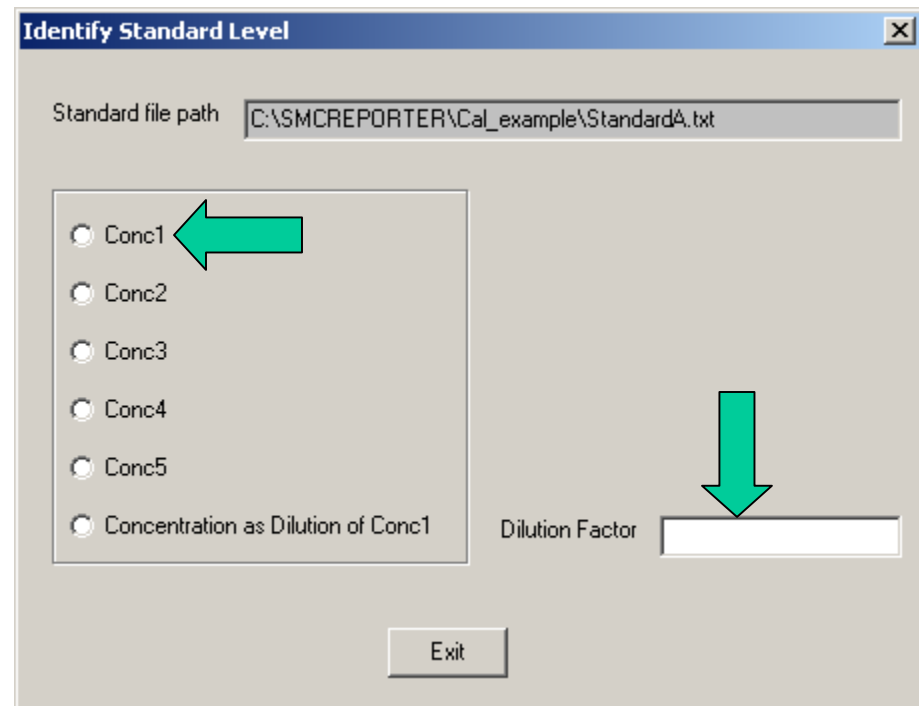
## Add Standard “A”

- Using the “Open” window navigate to the Cal\_example folder and select the file StandardA.txt then open. This file is the standard “A” listed in slide #9. Click “Open.”



# Adding Standards

- The Identify Standard Level window is displayed
- Select Conc1 or enter 1 in the Dilution factor field
- If a dilution factor is entered the Concentration as Dilution of Conc1 is automatically toggled.
- Select Exit to enter



## Create Calibration File with Standard A Added

- If there was an error in entry, highlight the standard file in the Data Directory and press “Delete” and repeat the Add Standard routine

**Create Calibration File**

Compound Library: C:\SMCREPORTER\CAL\_EXAMPLE\ALL.TXT

Surrogate Library: C:\SMCREPORTER\CAL\_EXAMPLE\SURROGATE.INI

Data Directory	Concentration
C:\SMCREPORTER\Cal_example\StandardA.txt	Conc1

Surrogate Reference: C:\SMCREPORTER\Cal\_example\blank.txt

☐ DO NOT print Surrogate report



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## Add Standards B-E

- Repeat the “Add Standard” routine for standards B-E. The dilutions for these standards are (0.2, 0.1, 0.06, and 0.02 respectively.
- The Create Calibration File should appear as

**Create Calibration File**

Compound Library: C:\SMCREPORTER\CAL\_EXAMPLE\ALL.TXT

Surrogate Library: C:\SMCREPORTER\CAL\_EXAMPLE\SURROGATE.INI

Data Directory	Concentration
C:\SMCREPORTER\Cal_example\StandardA.txt	Conc1
C:\SMCREPORTER\Cal_example\StandardB.txt	0.2
C:\SMCREPORTER\Cal_example\StandardC.txt	0.1
C:\SMCREPORTER\Cal_example\StandardD.txt	0.06
C:\SMCREPORTER\Cal_example\StandardE.txt	0.02

Surrogate Reference: C:\SMCREPORTER\Cal\_example\Blank.txt

☐ DO NOT print Surrogate report



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# *Review calibration curve*

- If all entries are correct the next step is to review the data.
- Press the “Review” tab on the “Create Calibration File” form.
- The following slide presents the “Review Calibration” form, starting at the first library entry ( the default).
- Note that no sample sizes are entered. Only the total ngs are being displayed. This is an important feature of method 8261 feature in that calibrations are by mass and not by matrix or sample size.



# Review Calibration Form

**Review Calibration**

Record Number:  Compound:

<-Previous

Calibration File:

Surrogate File:

	Std1	Std2	Std3	Std4	Std5	Reference file
Standard File Name	<input type="text" value="StandardA.t"/>	<input type="text" value="StandardB.t"/>	<input type="text" value="StandardC.t"/>	<input type="text" value="StandardD.t"/>	<input type="text" value="StandardE.t"/>	<input type="text" value="Blank.txt"/>
Concentrations	<input type="text" value="250"/>	<input type="text" value="250"/>	<input type="text" value="250"/>	<input type="text" value="250"/>	<input type="text" value="250"/>	
Recoveries (%)	<input type="text" value="76.888"/>	<input type="text" value="67.106"/>	<input type="text" value="82.001"/>	<input type="text" value="56.122"/>	<input type="text" value="65.346"/>	
Recovery (Dev.)	<input type="text" value="0.180"/>	<input type="text" value="0.040"/>	<input type="text" value="0.232"/>	<input type="text" value="0.059"/>	<input type="text" value="0.040"/>	
Area	<input type="text" value="184237"/>	<input type="text" value="198257"/>	<input type="text" value="195790"/>	<input type="text" value="157423"/>	<input type="text" value="198000"/>	
Response Factors	<input type="text" value="958.476"/>	<input type="text" value="1181.763"/>	<input type="text" value="955.067"/>	<input type="text" value="1121.999"/>	<input type="text" value="1212.003"/>	
Response Factor(Dev.)	<input type="text" value="224.187"/>	<input type="text" value="71.268"/>	<input type="text" value="270.407"/>	<input type="text" value="117.823"/>	<input type="text" value="74.892"/>	
Standard Included	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
Curve response factors	Standard Levels		Average	Deviation	% Deviation	
Average	<input type="text" value="(250, 250, 250, 250, 250)"/>		<input type="text" value="1085.862"/>	<input type="text" value="122.218"/>	<input type="text" value="11.255"/>	

☐ DO NOT Print Surrogate Report

☐ DO NOT Include Surrogate information on Calibration report



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# *Reviewing Calibration by Compound*

- By selecting the “Next” tab (upper left corner) each compound is displayed.
- An experimental surrogate, aniline- $^{13}\text{C}_6$ , was used in this calibration. This surrogate is not present in the available surrogate mix.
- Lets review the results for vinyl chloride. This can be done by entering “33” in the upper left corner record number box or clicking “next” to advance to 33.



# Eliminating a Data Point

**Review Calibration**

Record Number:  Compound:

<Previous Next>

Library File:

Calibration File:  Surrogate File:

acetophenone-d5  
1,2,4-trichlorobenzene-d3  
naphthalene-d8  
1-methylnaphthalene-d10  
dichlorodifluoromethane  
chloromethane  
**vinylchloride**

	Std1	Std2	Std3	Std4	Std5	Reference file
Standard File Name	<input type="text" value="StandardA.t"/>	<input type="text" value="StandardB.t"/>	<input type="text" value="StandardC.t"/>	<input type="text" value="StandardD.t"/>	<input type="text" value="StandardE.t"/>	<input type="text" value="Blank.txt"/>
Concentrations	<input type="text" value="250"/>	<input type="text" value="50"/>	<input type="text" value="25"/>	<input type="text" value="15"/>	<input type="text" value="5"/>	
Recoveries (%)	<input type="text" value="78.658"/>	<input type="text" value="78.550"/>	<input type="text" value="74.026"/>	<input type="text" value="83.416"/>	<input type="text" value="88.592"/>	
Recovery (Dev.)	<input type="text" value="0.003"/>	<input type="text" value="0.006"/>	<input type="text" value="0.000"/>	<input type="text" value="0.005"/>	<input type="text" value="0.006"/>	
Area	<input type="text" value="619683"/>	<input type="text" value="137239"/>	<input type="text" value="70641"/>	<input type="text" value="53310"/>	<input type="text" value="29993"/>	
Response Factors	<input type="text" value="3151.262"/>	<input type="text" value="3494.310"/>	<input type="text" value="3817.110"/>	<input type="text" value="4260.560"/>	<input type="text" value="6771.028"/>	
Response Factor(Dev.)	<input type="text" value="12.744"/>	<input type="text" value="27.888"/>	<input type="text" value="0.684"/>	<input type="text" value="27.354"/>	<input type="text" value="45.984"/>	
Standard Included	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
Curve response factors	Standard Levels		Average	Deviation	% Deviation	
Average	<input type="text" value="(250, 50, 25, 15, 5)"/>		<input type="text" value="4298.854"/>	<input type="text" value="1441.306"/>	<input type="text" value="33.528"/>	

Print ☐ DO NOT Print Surrogate Report ☐ DO NOT Include Surrogate information on Calibration report Save As Exit Help



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# *Editing the Calibration Curve*

- The large deviation for vinyl chloride (see lower arrow on previous slide) indicates there is a problem with vinyl chloride.
- We can see that the lower standard (StandardE, 5ngs) has a much larger response factor than the other four standards. Evaluating the chromatogram for vinyl chloride for that compound we found that low level interference was causing the bias.
- For this exercise we will assume that the lower amount of vinyl chloride is below all required limits and the standard data point is not necessary. Remove the “Standard Included” check on Standard E by clicking on it (see upper arrow on previous slide).
- By removing the data point the linearity will be recalculated. Also the change will be recorded in the calibration file and the lower calibration limit will become 15 ngs/sample.



# More Changes!

- The next two compounds that have large linearity deviations are common laboratory contaminants, Acetone (#38) and Methylene chloride (#43). The contribution due to background is observed in the elevated response factors for the lowest standards.
- For acetone remove data points for Standards D (30ng) and E (15 ng).
- For methylene chloride (#43) is also quite common. Remove data point for Standard E (5 ng/sample).
- Next advance to N-nitrosodimethylamine (#71). This compound chromatographs poorly on volatile organic compound capillary columns under most circumstances. (See next slide).



# N-Nitrosodimethylamine

**Review Calibration**

Record Number:  Compound:

<Previous

Calibration File:

Surrogate File:

Standard File Name:

Concentrations:

Recoveries (%):

Recovery (Dev.):

Area:

Response Factors:

Response Factor(Dev.):

Standard Included: ☒ ☒ ☒ ☒ ☒

Curve response factors: Standard Levels Average Deviation % Deviation

Average:

Print ☐ DO NOT Print Surrogate Report

☐ DO NOT Include Surrogate information on Calibration report



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## *N-Nitrosodimethylamine (cont)*

- Here, only the most concentrated standard (A) gives a response for the compound.
- Remove the “Standard Included” checks for standards B-E. This gives only a single data point. Other systems may give wider calibration range for this compound.
- Similarly, 2-picoline (#77), n-nitrosomethylethylamine (#82) and n-nitrosodipropylamine should be edited to give a single point.
- Aniline (#102) co-elutes with aniline- $^{13}\text{C}_6$  and the lower calibration levels are obscured by the surrogate. The two lower points should be removed. In the absence of the experimental co-eluting surrogate, calibration should be improved.



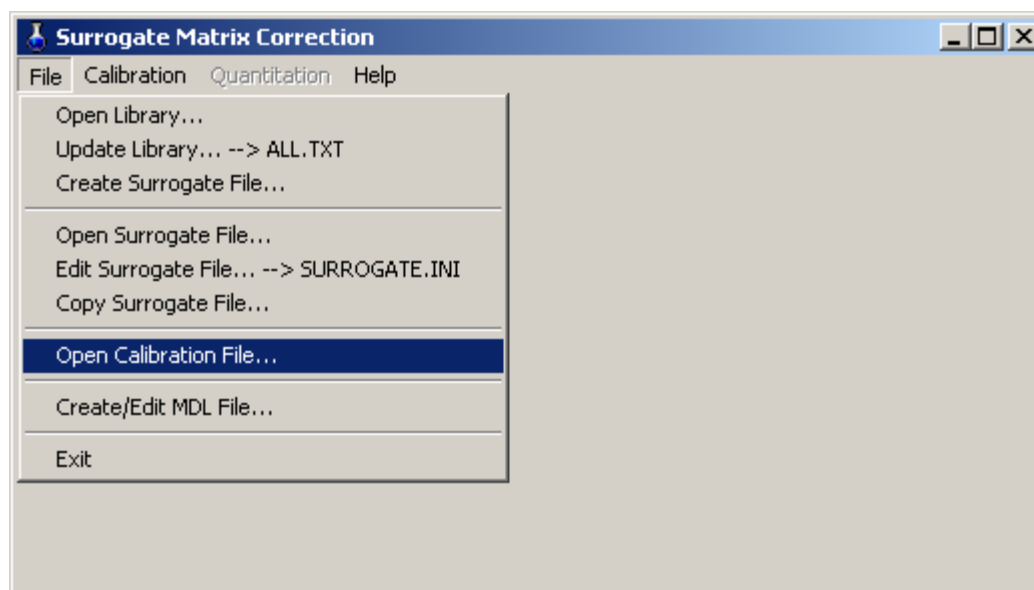
## *Save calibration curve*

- After the review, save the calibration curve. Click on the “Save as” button on the lower right hand corner of the review and save the file as “test.cal”.
- The calibration file is a standalone file containing all information necessary to process sample data. If the SMCReporter program is closed test.cal can be reloaded for sample processing. “All.txt” and “surrogate.ini” do not have to be recalled.



# Quantitate samples

- The newly created calibration file can now be used to process data.
- Load the calibration file by File->Open Calibration File



- Select the newly created test.cal



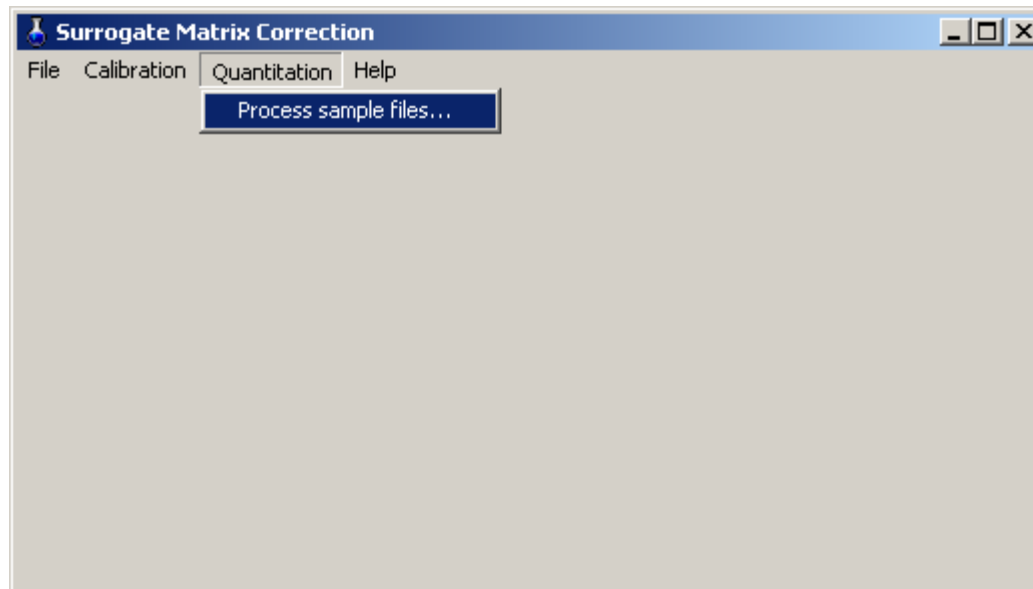
# *Calibration Loaded*

- Notice that after loading the calibration file that library All.txt and surrogate.ini are disabled (under File).
- The main window (see slide 4) now has Calibration and Quantitation menu options enabled.
- In the Calibration menu options for review, printing, and check standard reporting are now enabled.



# Quantitation

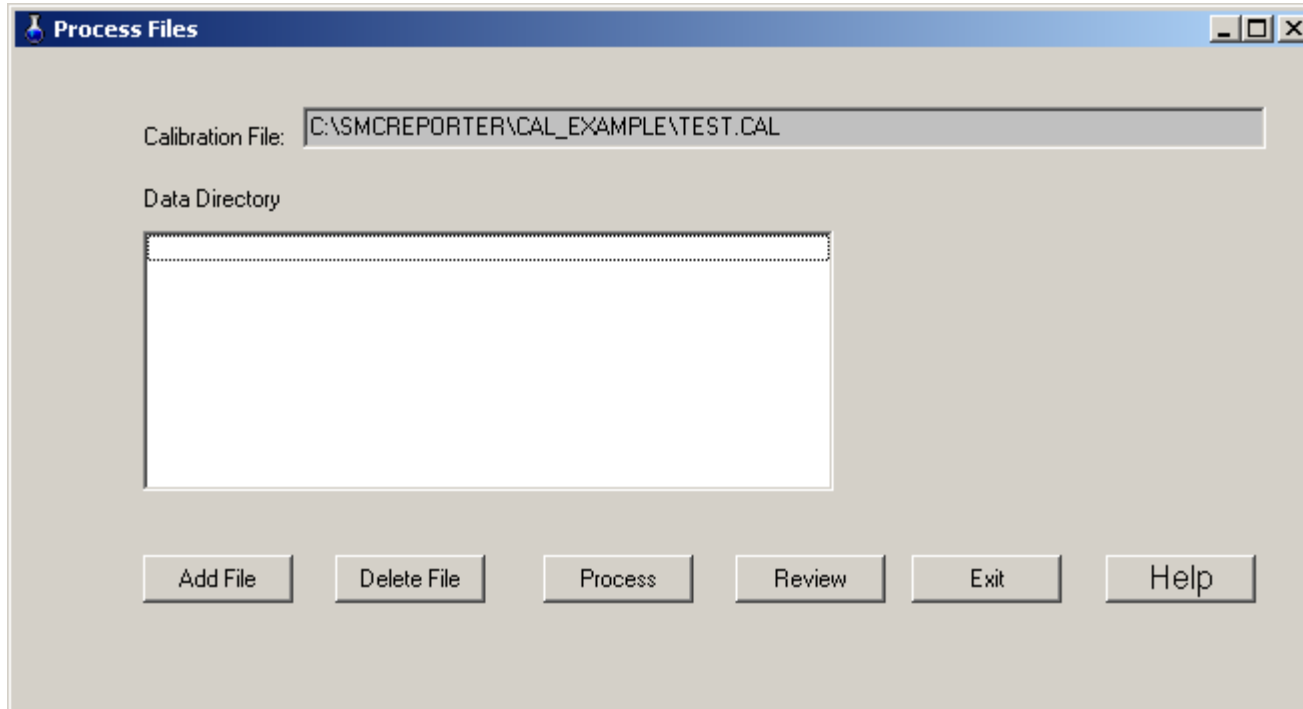
- With calibration file test.cal loaded the next step is to start the quantitation process.
- Select Quantitation->Process Sample Files



- The Process Files window for entering samples appears (next slide).



# Enter File for Quantitation



- Select “Add File” and navigate to the blank used in calibration (Blank.txt)
- Upon selection of file a window for inputting sample information appears (next slide).



# *Input Window for File Processing*

**File Processing Input**

Current Sample File:

Method Detection Limits

List MDL

☒ No

☐ Yes

Reporting Units:

Sample Size:

Matrix:

Other:

DO NOT Print Surrogate report ☐

Comment 1:

Comment 2:



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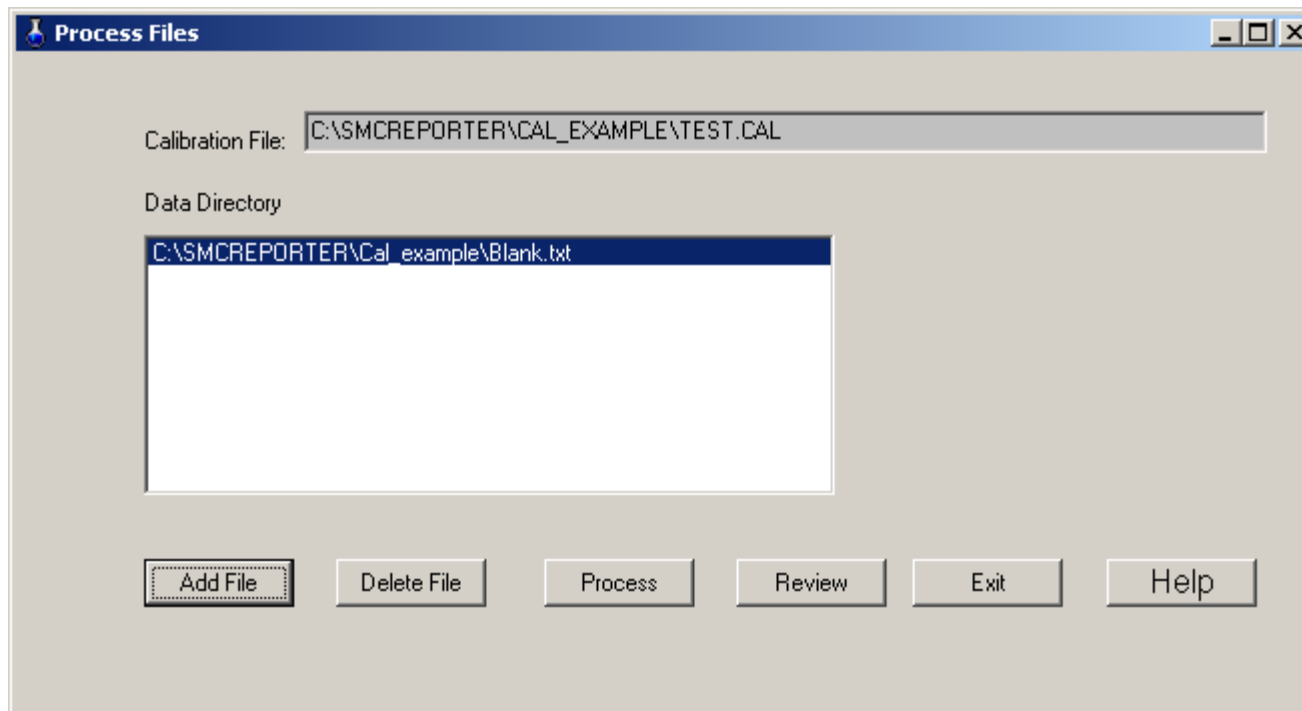
# Sample Information

- Leave the “List MDL” “no” checked.
- Leave the reporting units as ng/mL.
- Enter 5 for the sample size (5 mL).
- Enter “Water” for matrix.
- The fields “other”, and “comments” 1 and 2 are for entering sample specific data.
- Check the “DO NOT print surrogate report” box. We will address that report later.
- Click “Enter”. The next window should look like the following slide.





# Sample Ready to Process

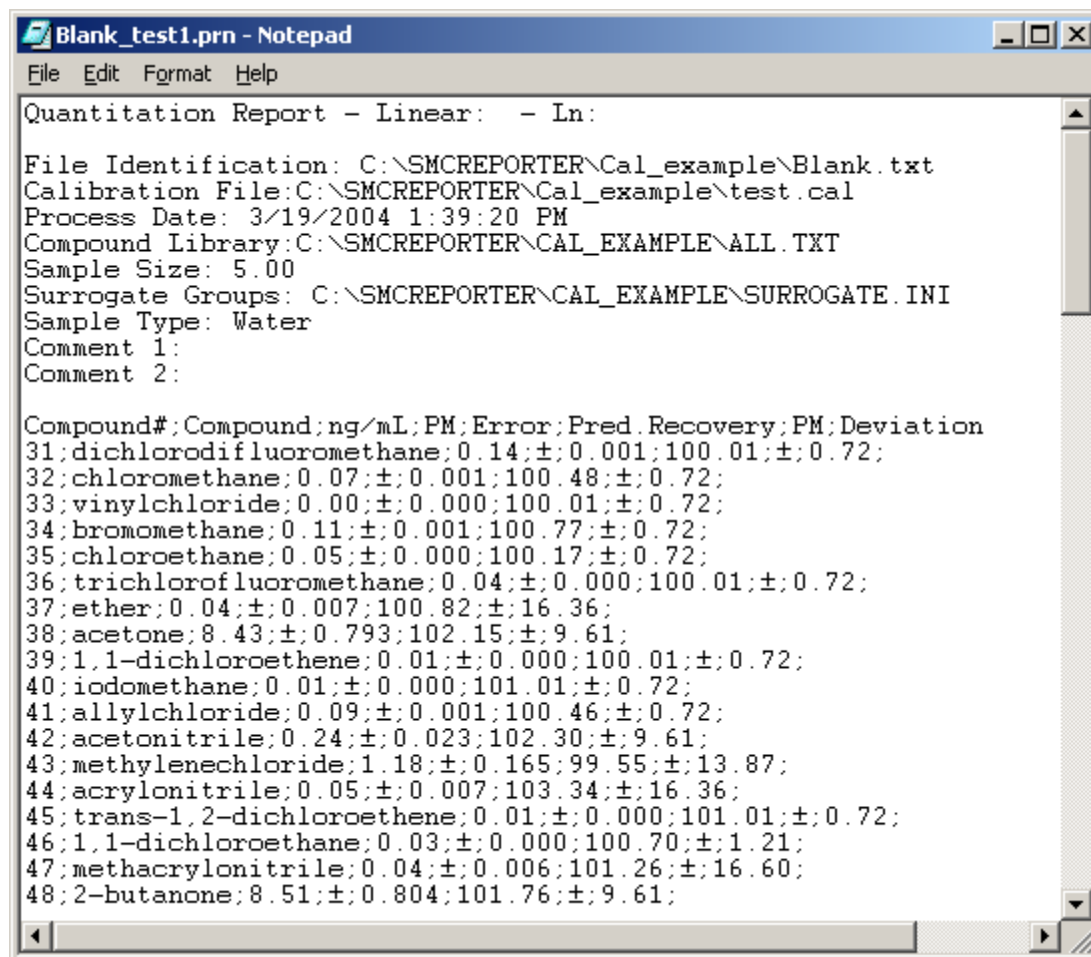


- For this exercise we will only process the blank. The standard runs can also be quantitated like samples if desired.
- Now click “Process” and a quantitation report (both paper and electronic) will be generated for the sample.



# Electronic Data Report

- The file name of the report is Blank\_test1.prn and resides in the same folder Blank.txt resides. The “test1” represents the calibration “test.cal” and the first quantitation of the file using test.cal.



```
Blank_test1.prn - Notepad
File Edit Format Help
Quantitation Report - Linear: - Ln:

File Identification: C:\SMCREPORTER\Cal_example\Blank.txt
Calibration File: C:\SMCREPORTER\Cal_example\test.cal
Process Date: 3/19/2004 1:39:20 PM
Compound Library: C:\SMCREPORTER\CAL_EXAMPLE\ALL.TXT
Sample Size: 5.00
Surrogate Groups: C:\SMCREPORTER\CAL_EXAMPLE\SURROGATE.INI
Sample Type: Water
Comment 1:
Comment 2:

Compound#:Compound;ng/mL;PM;Error;Pred.Recovery;PM;Deviation
31;dichlorodifluoromethane;0.14;±0.001;100.01;±0.72;
32;chloromethane;0.07;±0.001;100.48;±0.72;
33;vinylchloride;0.00;±0.000;100.01;±0.72;
34;bromomethane;0.11;±0.001;100.77;±0.72;
35;chloroethane;0.05;±0.000;100.17;±0.72;
36;trichlorofluoromethane;0.04;±0.000;100.01;±0.72;
37;ether;0.04;±0.007;100.82;±16.36;
38;acetone;8.43;±0.793;102.15;±9.61;
39;1,1-dichloroethene;0.01;±0.000;100.01;±0.72;
40;iodomethane;0.01;±0.000;101.01;±0.72;
41;allylchloride;0.09;±0.001;100.46;±0.72;
42;acetonitrile;0.24;±0.023;102.30;±9.61;
43;methylenechloride;1.18;±0.165;99.55;±13.87;
44;acrylonitrile;0.05;±0.007;103.34;±16.36;
45;trans-1,2-dichloroethene;0.01;±0.000;101.01;±0.72;
46;1,1-dichloroethane;0.03;±0.000;100.70;±1.21;
47;methacrylonitrile;0.04;±0.006;101.26;±16.60;
48;2-butanone;8.51;±0.804;101.76;±9.61;
```



# *Quantitation Report*

- Note the header contains a description of all components that were used to generate the report and the file path.
- Each compound is listed with its calculated concentration, method error, predicted recovery and deviation.
- The paper copy of the report contains the same information but with a presentation more compatible with a paper display.
- Normally results are not reported if they do not exceed some limit such as method detection limit (MDL). addressed in the following slide.



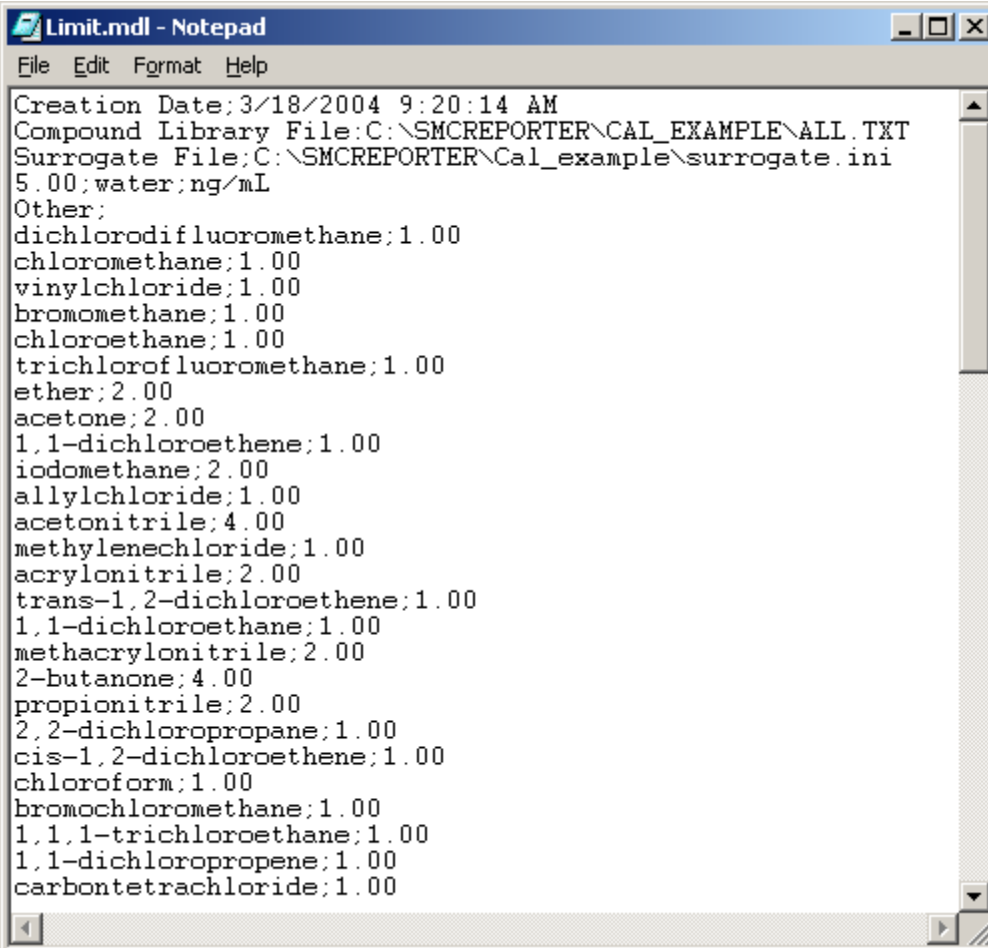
# MDL data

- The MDL option on the File Processing Input window (slide #31) is the means to limit results to only those above a threshold (method detection limit, reporting limit, lower calibration point).
- A limit file was created for this presentation as the the concentration of the lower calibration point in 5 mL water (Limit.mdl).
- The adventurous can create their own limit file. This requires reloading the library, All.txt, and the surrogate file, surrogate.ini. Then Menu->File->Create/Edit MDL File. Type of limit file (matrix and sample size) are entered and compound limits be entered individually or through a paste command. See the SMCReporter operating manual for greater detail.
- The next slide presents the format of the file (Limit.mdl).



# Limit.txt

- The limit file is a “;” delimited \*.mdl file.
- The header contains information to identify what sample size, matrix, library and surrogate are related to the limit.
- Labeling limit files should include pertinent information such as “5mLwatermdl\_inst1.mdl” or “5mLreportlimit.mdl” for ease of locating.



```
Limit.mdl - Notepad
File Edit Format Help
Creation Date;3/18/2004 9:20:14 AM
Compound Library File;C:\SMCREPORTER\CAL_EXAMPLE\ALL.TXT
Surrogate File;C:\SMCREPORTER\Cal_example\surrogate.ini
5.00;water;ng/mL
Other;
dichlorodifluoromethane;1.00
chloromethane;1.00
vinylchloride;1.00
bromomethane;1.00
chloroethane;1.00
trichlorofluoromethane;1.00
ether;2.00
acetone;2.00
1,1-dichloroethene;1.00
iodomethane;2.00
allylchloride;1.00
acetonitrile;4.00
methylenechloride;1.00
acrylonitrile;2.00
trans-1,2-dichloroethene;1.00
1,1-dichloroethane;1.00
methacrylonitrile;2.00
2-butanone;4.00
propionitrile;2.00
2,2-dichloropropane;1.00
cis-1,2-dichloroethene;1.00
chloroform;1.00
bromochloromethane;1.00
1,1,1-trichloroethane;1.00
1,1-dichloropropene;1.00
carbontetrachloride;1.00
```



## *Process Files with a Reporting Limit*

- To observe the use of limits return to the data processing routine (slide 29) and re-enter the Blank.txt. When the “File Processing Input” window is displayed check “yes” in the “List MDL” option.
- Note that the window retains the previous inputs as new defaults.



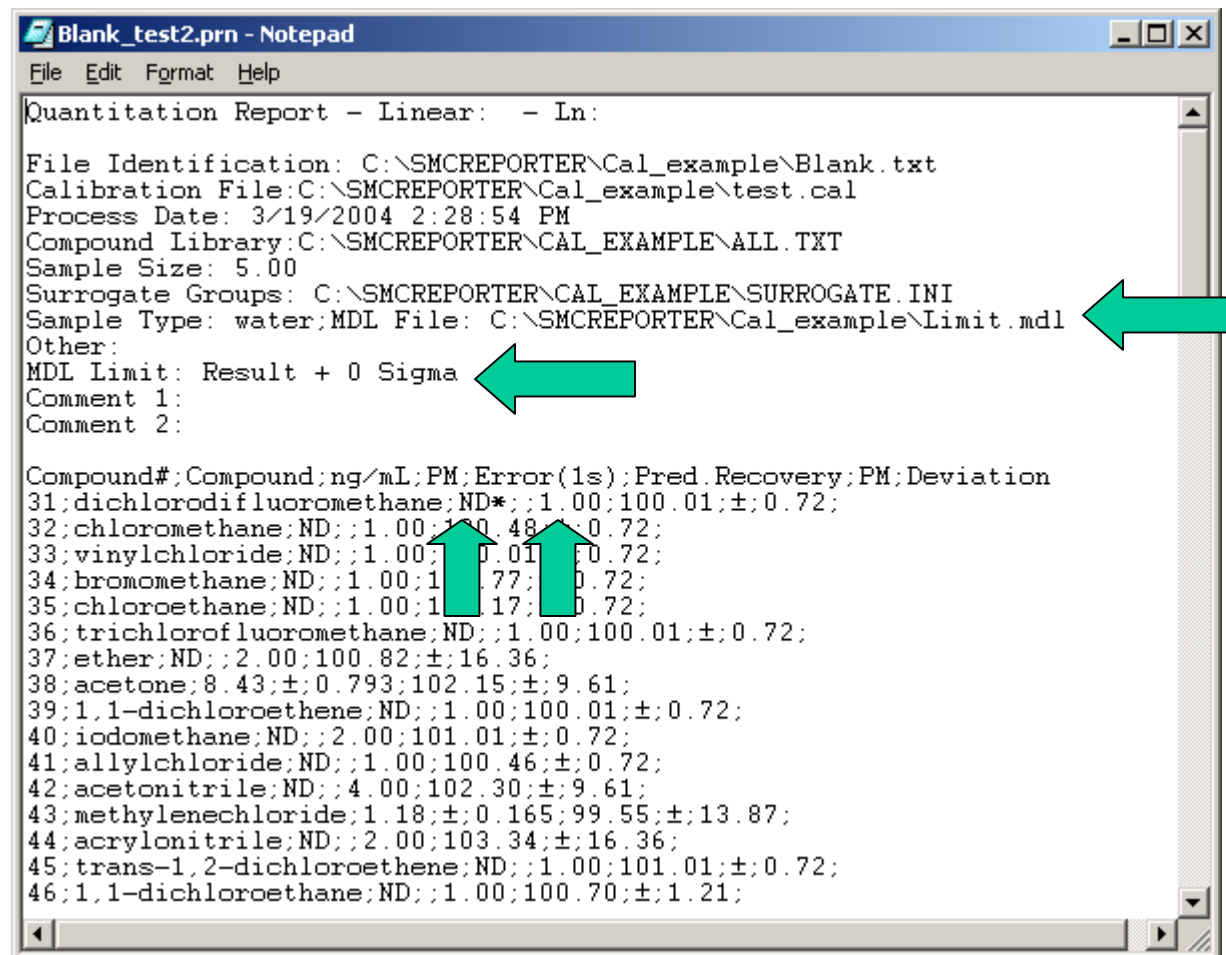
## Input with Limit Option

- Use browse to locate the MDL file “Limit.mdl” and load.
- The “DO NOT Print Surrogate report” should not be checked. We will look at the surrogate files this time.
- For now the “Reporting Limits” box remains “0”.
- Click “Enter”.
- Then click “Process” on the returned Process Files window.

The screenshot shows the 'File Processing Input' dialog box. At the top, the 'Current Sample File' is set to 'C:\SMCREPORTER\CAL\_EXAMPLE\BLANK.TXT'. Below this, the 'Method Detection Limits' section contains a 'List MDL' group box with 'No' and 'Yes' radio buttons (the 'Yes' button is selected). To the right of this group box is a 'Reporting Limits (Number of Standard Deviations)' dropdown menu currently set to '0'. A green arrow points up to this dropdown. Below the 'List MDL' group box is a 'Browse for MDL File' button, with a green arrow pointing to it. Further down, there are input fields for 'Reporting Units' (set to 'ng/mL'), 'Sample Size' (set to '5'), 'Matrix' (set to 'Water'), and 'Other' (empty). At the bottom of the dialog, there is a checkbox labeled 'DO NOT Print Surrogate report' which is unchecked, with a green arrow pointing to it. Below the checkbox are two text input fields for 'Comment 1' and 'Comment 2'. At the very bottom are 'Enter' and 'Help' buttons.



# Electronic Data Report with Limits



Blank\_test2.prn - Notepad

File Edit Format Help

Quantitation Report - Linear: - Ln:

File Identification: C:\SMCREPORTER\Cal\_example\Blank.txt  
Calibration File: C:\SMCREPORTER\Cal\_example\test.cal  
Process Date: 3/19/2004 2:28:54 PM  
Compound Library: C:\SMCREPORTER\CAL\_EXAMPLE\ALL.TXT  
Sample Size: 5.00  
Surrogate Groups: C:\SMCREPORTER\CAL\_EXAMPLE\SURROGATE.INI  
Sample Type: water; MDL File: C:\SMCREPORTER\Cal\_example\Limit.md1  
Other:  
MDL Limit: Result + 0 Sigma  
Comment 1:  
Comment 2:

Compound#; Compound; ng/mL; PM; Error(1s); Pred. Recovery; PM; Deviation

31;	dichlorodifluoromethane;	ND*;;	1.00;	100.01;	±0.72;		
32;	chloromethane;	ND;;	1.00;	100.48;	±0.72;		
33;	vinylchloride;	ND;;	1.00;	100.01;	±0.72;		
34;	bromomethane;	ND;;	1.00;	100.77;	±0.72;		
35;	chloroethane;	ND;;	1.00;	100.17;	±0.72;		
36;	trichlorofluoromethane;	ND;;	1.00;	100.01;	±0.72;		
37;	ether;	ND;;	2.00;	100.82;	±16.36;		
38;	acetone;	8.43;	±0.793;	102.15;	±9.61;		
39;	1,1-dichloroethene;	ND;;	1.00;	100.01;	±0.72;		
40;	iodomethane;	ND;;	2.00;	101.01;	±0.72;		
41;	allylchloride;	ND;;	1.00;	100.46;	±0.72;		
42;	acetonitrile;	ND;;	4.00;	102.30;	±9.61;		
43;	methylenechloride;	1.18;	±0.165;	99.55;	±13.87;		
44;	acrylonitrile;	ND;;	2.00;	103.34;	±16.36;		
45;	trans-1,2-dichloroethene;	ND;;	1.00;	101.01;	±0.72;		
46;	1,1-dichloroethane;	ND;;	1.00;	100.70;	±1.21;		





# *Quantitation Report with Limits*

- The electronic version name is Blank\_test2.prn with the “2” indicating this is the second quantitation of the file using test.cal.
- The reprocessed quantitation report now displays the results with “ND” for not detected below the limit (Limit.mdl is in the header)
- The limit values are now presented in the “Error” column.
- The paper version of the report contains the same information as the new electronic version but in a different layout as before.



# Reporting Limits Including Method Precision

- Note that in the header there is a MDL limit: with “Result + 0 Sigma”. This is the “0” value in “Reporting Limits (number of standard deviations)” from the File Process Input window. This value is included in reporting values and including the method error. If “3” is entered in the input window, a compound concentration will be reported if the upper limit of 3x the method error is  $\geq$  the limit.
- Reprocess the Blank.txt file with the reporting limits deviation at “3”. **Note: the method error reported with concentrations is still only 1 deviation.**
- A concentration (in ng/mL) for aniline will be displayed as  $45.6 \pm 6.47$  and not “ND”. This is because the aniline concentration + 3Xdeviation exceed the limit ( $45.6 + 3 \times 6.47 = 65.01 > \text{the 60 limit value}$ ).



# QC report

- The QC report contains the equations used to generate the results (paper copy presents a graphic presentation of effects observed).
- The QC report contains the method 8261 calculations on the monitoring “check” surrogates as individual compounds and as volatile, non-purgeable volatile, and semivolatile groupings.
- With the exception of graphics the electronic version of the QC report contains the same data and this discussion will reference the electronic version.

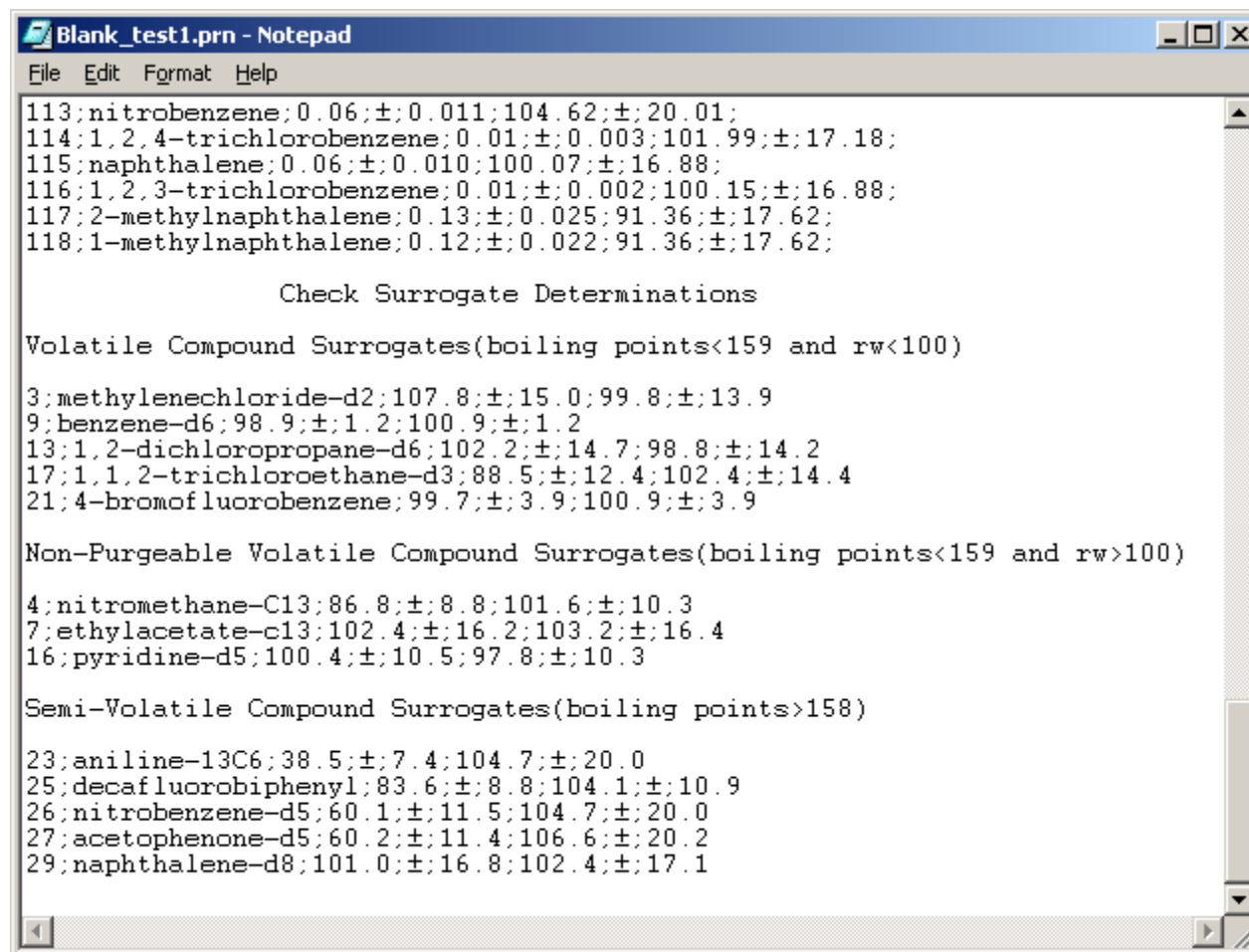


# *Electronic QC Report*

- The check surrogates are presented following the listing of the compound results in the data file. See next slide. The check surrogate results are also presented in a separate QC file.
- The electronic QC report is included in a \*.SQL file. To read the file use notepad and open Blank\_test2.SQC.
- The Blank\_test2.SQL file is displayed in the slide #46.



# Electronic Version of Check Surrogates



```
Blank_test1.prn - Notepad
File Edit Format Help
113;nitrobenzene;0.06;±;0.011;104.62;±;20.01;
114;1,2,4-trichlorobenzene;0.01;±;0.003;101.99;±;17.18;
115;naphthalene;0.06;±;0.010;100.07;±;16.88;
116;1,2,3-trichlorobenzene;0.01;±;0.002;100.15;±;16.88;
117;2-methylnaphthalene;0.13;±;0.025;91.36;±;17.62;
118;1-methylnaphthalene;0.12;±;0.022;91.36;±;17.62;

Check Surrogate Determinations

Volatile Compound Surrogates(boiling points<159 and rw<100)

3;methylenechloride-d2;107.8;±;15.0;99.8;±;13.9
9;benzene-d6;98.9;±;1.2;100.9;±;1.2
13;1,2-dichloropropane-d6;102.2;±;14.7;98.8;±;14.2
17;1,1,2-trichloroethane-d3;88.5;±;12.4;102.4;±;14.4
21;4-bromofluorobenzene;99.7;±;3.9;100.9;±;3.9

Non-Purgeable Volatile Compound Surrogates(boiling points<159 and rw>100)

4;nitromethane-C13;86.8;±;8.8;101.6;±;10.3
7;ethylacetate-c13;102.4;±;16.2;103.2;±;16.4
16;pyridine-d5;100.4;±;10.5;97.8;±;10.3

Semi-Volatile Compound Surrogates(boiling points>158)

23;aniline-13C6;38.5;±;7.4;104.7;±;20.0
25;decafluorobiphenyl;83.6;±;8.8;104.1;±;10.9
26;nitrobenzene-d5;60.1;±;11.5;104.7;±;20.0
27;acetophenone-d5;60.2;±;11.4;106.6;±;20.2
29;naphthalene-d8;101.0;±;16.8;102.4;±;17.1
```



# QC Report-Electronic Format

```
Blank_test2.SQC - Notepad
File Edit Format Help

Surrogate Report
Process Date:3/19/2004 2:28:54 PM
Compound Library File:C:\SMCREPORTER\CAL_EXAMPLE\ALL.TXT
Surrogate Groupings File:C:\SMCREPORTER\CAL_EXAMPLE\SURROGATE.INI
C:\SMCREPORTER\CAL_EXAMPLE\BLANK.TXT
Calibration File:C:\SMCREPORTER\Cal_example\test.cal

First Pass relative Volatility (Ln) vs. Recovery
(Used to Estimate Rel vol effects on BP Surrogates)

Compound;; Measured; Recovery
hexafluorobenzene;81.5;0.86;99.98;99.98
Fluorobenzene;85.0;3.50;100.38;100.38

Slope = 0.002884; Intercept = 1.000215; Error = 0.000; RSQ = 0.000000

Fluorobenzene;85.0;3.50;100.38;100.38
1,2-dichloroethane-d4;84.0;20.00;95.27;95.27

Slope = -0.029346; Intercept = 1.040591; Error = 0.000; RSQ = 0.000000

Recovery vs. Boiling Point - (First Pass Rel Vol Corrections)-- Boiling point range( 85.00 - 231.00)
Compound;; Measured; Recovery
pentafluorobenzene;85.0;1.51;100.49;100.35
toluene-d8;111.0;4.28;96.49;96.70
bromobenzene-d5;155.0;7.93;100.91;102.99

Slope = 0.000488; Intercept = 0.943014; Error = 0.037; RSQ = 0.000011

bromobenzene-d5;155.0;7.93;100.91;102.99
```



## Summary

- All data is generated in paper and electronic format.
- QC is generated for each sample.
- There are options for limits to report data.
- Data generated can be read into other programs for customizing reports.

**Note: The SMCReporter will be updated periodically to add new features.**

